

ABSTRACT OF THE DISCLOSURE

A method, system, and computer program product for mining mass spectral data to detect chemical-specific characteristic features in large databases and/or files, including specifying spectral characteristics of mass spectra to mine, specifying a relationship between the spectral characteristics, searching the mass spectra for portions of the mass spectra which match the spectral characteristics based on the relationship, and assigning scores to the portions of mass spectra to indicate a degree of correlation between the portions of mass spectra and the spectral characteristics. Exemplary embodiments encompass a user specification of the spectral characteristics and their relationships used to mine the mass spectral data, automated specification of the spectral characteristics and their relationships used to mine the data, and real-time data mining wherein the mass spectrometer is adjusted based on the result.